

# Supplementary Information

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**Table S1.**  $^1\text{H}$  (600 MHz) and  $^{13}\text{C}$  (150 MHz) NMR chemical shifts (DMSO- $d_6$  and  $\text{CD}_3\text{OD}$ ), NOESY and HMBC correlations of compound **1**.

No.	DMSO- $d_6$		$\text{CD}_3\text{OD}$		NOESY	DMSO- $d_6$	$\text{CD}_3\text{OD}$	Type	HMBC ( $^{13}\text{C} \rightarrow ^1\text{H}$ )
	$^1\text{H}$ ( $\delta$ )	m (J)	$^1\text{H}$ ( $\delta$ )	m (J)		$^{13}\text{C}$ ( $\delta$ )	$^{13}\text{C}$ ( $\delta$ )		
1	$\beta$ 1.59	m	$\beta$ 1.73	m	11 $\beta$	35.8	37.4	$\text{CH}_2$	19
	$\alpha$ 1.03	m	$\alpha$ 1.18	m	2 $\alpha$ , 3				
2	$\alpha$ 2.10	m	$\alpha$ 2.26	m	1 $\alpha$ , 1 $\beta$ , 3	28.2	29.4	$\text{CH}_2$	
	$\beta$ 1.28	m	$\beta$ 1.56	m	19				
3	3.53	ddd 10.9, 10.9, 4.4	3.86	ddd 11.0, 10.6, 4.8	1 $\alpha$ , 2 $\alpha$ , 5, 29	80.1	85.2	CH	4, 29
4	1.21	m	1.44	m	6 $\beta$ , 19	37.2	38.9	CH	29
5	0.87	m	0.97	m	3, 9	50.7	52.6	CH	1 $\beta$ , 4, 6 $\beta$ , 7 $\beta$ , 19, 29
6	$\alpha$ 1.65	m	$\alpha$ 1.77	m	4, 7 $\beta$	24.7	26.2	$\text{CH}_2$	5, 7 $\alpha$
	$\beta$ 0.90	m	$\beta$ 1.02	m					
7	$\beta$ 2.32	br. dd 12.6, 3.7	$\beta$ 2.44	m	6 $\beta$ , 15 $\alpha$ , 15 $\beta$	29.2	30.7	$\text{CH}_2$	
	$\alpha$ 1.65	m	$\alpha$ 1.73	m	15 $\alpha$				
8	-		-			125.9	127.4	C	6 $\alpha$ , 7 $\beta$ , 9, 15 $\beta$
9	1.61	m	1.08	m	5, 12 $\alpha$	48.7	50.7	CH	7 $\beta$ , 11 $\alpha$ , 12 $\beta$ , 19
10	-		-			36.9	38.7	C	6 $\beta$ , 9, 19
11	$\alpha$ 1.55	m	$\alpha$ 1.61	m	12 $\alpha$ , 12 $\beta$	19.5	21.1	$\text{CH}_2$	9
	$\beta$ 1.41	m	$\beta$ 1.51	m	1 $\beta$ , 12 $\beta$ , 18				
12	$\beta$ 1.87	ddd 12.2, 3.2, 3.2	$\beta$ 1.93	ddd 12.2, 3.4, 3.3	11 $\alpha$ , 11 $\beta$ , 12 $\alpha$ ,	36.9	38.3	$\text{CH}_2$	9, 18
	$\alpha$ 1.04	m	$\alpha$ 1.09	m	17, 21 9, 11 $\alpha$				
13	-		-			42.2	43.8	C	11 $\beta$ , 15 $\beta$ , 16 $\alpha$ , 17, 18
14	-		-			141.4	143.3	C	7 $\alpha$ , 9, 12 $\beta$ , 15 $\alpha$ , 15 $\beta$ , 16 $\alpha$ , 16 $\beta$ , 18
15	$\alpha$ 2.18	br. dd 16.7, 10.2	2.19	m	7 $\alpha$ , 7 $\beta$ , 16 $\alpha$ ,	25.3	26.6	$\text{CH}_2$	
	$\beta$ 2.11	m		m	16 $\beta$ 7 $\beta$ , 16 $\alpha$ , 16 $\beta$				
16	$\alpha$ 1.71	dddd 13.1, 9.6, 7.3, 2.3	$\alpha$ 1.74	m	15 $\alpha$ , 15 $\beta$ , 17	26.6	28.1	$\text{CH}_2$	15 $\beta$
	$\beta$ 1.28	m	$\beta$ 1.32	m	15 $\alpha$ , 15 $\beta$				
17	1.02	m	1.03	m	12 $\alpha$ , 16 $\alpha$ , 21	56.3	58.2	CH	15 $\alpha$ , 18, 20, 21
18	0.78	s	0.82	s	11 $\beta$ , 19, 20	18.1	18.7	$\text{CH}_3$	17
19	0.64	s	0.74	s	2 $\beta$ , 4, 18	13.7	14.4	$\text{CH}_3$	
20	1.37	m	1.39	m	18	34.1	35.9	CH	21, 23a
21	0.86	d 6.6	0.88	d 6.7	12 $\beta$ , 17	19.0	19.6	$\text{CH}_3$	23b
22	1.33	m	a 1.41	m	24	32.5	34.1	$\text{CH}_2$	21
	0.98	m	b 1.02	m					

Table S1. Cont.

23	1.48	12.0, 6.7, 4.3	a 1.51	m	24, 26b	31.3	33.4	CH <sub>2</sub>	24, 28
	1.15	dddd 12.0, 10.6, 6.6, 4.8	b 1.19	m	24				
24	2.50	m	2.62	ddq 7.0, 7.0, 7.0	22a, 23a, 23b	35.0	36.6	CH	23b, 26a, 26b, 28
25	-	-	-	-	-	151.4	152.7	C	23a, 23b, 24, 26a, 26b, 28
26	5.53	s	a 5.68	s	NH	113.9	115.8	CH <sub>2</sub>	24
	5.17	s	b 5.26	br. s	23a, 28				
27	-	-	-	-	-	166.7	170.3	C	24, 26a, 26b, 30, NH
28	0.99	d 6.9	1.08	d 6.9	26b	19.7	19.8	CH <sub>3</sub>	23a, 23b, 24
29	0.87	d 6.3	1.02	d 6.3	3	15.5	16.0	CH <sub>3</sub>	-
30	4.60	d 5.8	5.25	s	37	58.2	59.9	CH	33, 37, NH
31	-	-	-	-	-	170.4	173.3	C	30, NH
32	-	-	-	-	-	134.9	132.9	C	-
33	7.18	d 8.6	7.36	d 8.7	-	127.5	129.4	CH	30, 37
34	6.74	d 8.6	6.82	d 8.7	38	112.7	114.6	CH	33, 36
35	-	-	-	-	-	157.5	160.3	C	33, 34, 36, 37, 38
36	6.74	d 8.6	6.82	d 8.7	38	112.7	114.6	CH	34, 37
37	7.18	d 8.6	7.36	d 8.7	30, NH	127.5	129.4	CH	30, 33
38	3.67	s	3.75	s	34, 36	55.0	55.7	CH <sub>3</sub>	-
NH	7.78	d 5.8	-	-	26a, 37	-	-	-	-

Table S2. <sup>1</sup>H (600 MHz) and <sup>13</sup>C (150 MHz) NMR chemical shifts (DMSO-*d*<sub>6</sub> and CD<sub>3</sub>OD), NOESY and HMBC correlations of compound 2.

No.	DMSO- <i>d</i> <sub>6</sub>		CD <sub>3</sub> OD		NOESY	DMSO- <i>d</i> <sub>6</sub>	CD <sub>3</sub> OD	Type	HMBC ( <sup>13</sup> C→ <sup>1</sup> H)
	<sup>1</sup> H (δ)	m (J)	<sup>1</sup> H (δ)	m (J)		<sup>13</sup> C (δ)	<sup>13</sup> C (δ)		
1	β 1.56	m	β 1.71	ddd 13.3, 3.5, 3.5	2α, 2β, 19	35.6	37.2	CH <sub>2</sub>	2α, 19
	α 1.02	m	α 1.17	m	2α, 3, 5				
2	α 2.09	dm 12.2	α 2.27	m	1α, 1β, 3	28.1	29.3	CH <sub>2</sub>	1β
	β 1.28	m	β 1.56	m	1β, 19				
3	3.50	ddd 11.2, 10.0, 4.8	3.85	ddd 11.2, 10.0, 4.8	1α, 2α, 5, 29	80.2	85.1	CH	1β, 29
4	1.20	m	1.42	m	6β, 19, 29	36.8	38.4	CH	6β, 29, 5
5	1.22	m	1.38	ddd 11.5, 9.0, 2.5	1α, 3, 6α, 9, 29, 39	44.1	45.7	CH	1α, 4, 7, 19, 29
6	α 1.83	m	α 1.98	ddd 14.6, 2.9, 2.5	5, 39	30.4	31.4	CH <sub>2</sub>	5, 7
	β 1.07	m	β 1.20	m	4, 7, 19				
7	3.94	br. s	4.08	dd 2.9, 2.8	6β, 15β	73.3	75.6	CH	6α, 9, 39
8	-	-	-	-	-	124.5	125.8	C	6α, 9, 11β, 15α
9	1.87	m	1.95	m	5, 11α, 39	43.4	45.3	CH	1β, 7, 12β, 19
10	-	-	-	-	-	37.1	38.6	C	5, 6α, 9, 19
11	α 1.56	m	α 1.63	dddd 13.9, 7.5, 3.4,	9, 12α, 12β	19.8	20.5	CH <sub>2</sub>	9, 12β
	β 1.36	m	β 1.48	3.4 m	12β, 18, 19				

Table S2. Cont.

12	$\beta$ 1.89 $\alpha$ 1.04	m m	$\beta$ 1.96 $\alpha$ 1.12	m m	11 $\alpha$ , 11 $\beta$ , 18, 21 11 $\alpha$ , 39	36.6	38.2	CH <sub>2</sub>	9, 18
13	-		-			42.8	44.6	C	11 $\beta$ , 12 $\alpha$ , 15 $\alpha$ , 17, 18
14	-		-			147.9	150.6	C	7, 9, 12 $\beta$ , 15 $\alpha$ , 15 $\beta$ , 16 $\alpha$ , 16 $\beta$
15	$\alpha$ 2.37 $\beta$ 2.21	ddd 17.6, 9.5, 8.7 br. dd 17.6, 12.4	$\alpha$ 2.43 $\beta$ 2.25	ddd 17.6, 9.5, 8.7 m	16 $\alpha$ , 17, 39 7, 16 $\beta$ , 18	25.0	26.4	CH <sub>2</sub>	
16	$\alpha$ 1.76 $\beta$ 1.31	m m	$\alpha$ 1.80 $\beta$ 1.34	dddd 13.0, 9.5, 7.1, 2.3 m	15 $\alpha$ , 17, 22a, 22b 15 $\beta$ , 18	26.4	27.9	CH <sub>2</sub>	15 $\alpha$ , 17
17	1.05	m	1.10	m	15 $\alpha$ , 16 $\alpha$ , 21	56.6	58.4	CH	16 $\beta$ , 18, 21, 20, 22a, 22b
18	0.80	s	0.85	s	11 $\beta$ , 12 $\beta$ , 15 $\beta$ , 16 $\beta$ , 20	17.4	18.1	CH <sub>3</sub>	12 $\alpha$
19	0.63	s	0.74	s	1 $\beta$ , 2 $\beta$ , 4, 6 $\beta$ , 11 $\beta$	12.9	13.6	CH <sub>3</sub>	1 $\alpha$
20	1.38	m	1.41	m	18, 21	34.1	35.8	CH	21, 22b, 23a
21	0.89	d 6.4	0.91	d 6.6	12 $\beta$ , 17, 20, 23b	19.0	19.6	CH <sub>3</sub>	
22	a1.36 b0.97	m m	a1.41 b1.02	m m	16 $\alpha$ , 24, 28 16 $\alpha$ , 23a	32.5	33.9	CH <sub>2</sub>	20, 21, 23b, 24
23	a1.49 b1.17	m m	a1.53 b1.22	m m	22b, 24, 26b, 28 21, 24, 26b	31.5	33.3	CH <sub>2</sub>	24, 28, 20, 22a
24	2.50	m	2.62	ddq 6.5, 6.5, 6.5	22a, 23a, 23b, 26b, 28	35.0	36.5	CH	23a, 23b, 26a, 26b, 28
25	-		-			151.3	152.6	C	23a, 23b, 24, 26a, 26b, 28
26	a5.53 b5.17	s br. s	a5.69 b5.27	s br. s	23a, 23b, 24, 28	114.0	116.0	CH <sub>2</sub>	24
27	-		-			166.7	170.9	C	26a, 26b, NH
28	1.00	d 6.9	1.08	d 6.9	22a, 23a, 24, 26b	19.0	20.0	CH <sub>3</sub>	24
29	0.84	d 5.8	1.01	d 6.0	3, 4, 5	15.4	15.8	CH <sub>3</sub>	5
30	4.57	d 5.0	5.24	s	33, 37	58.2	59.9	CH	33, 37, NH
31	-		-			170.5	176.8	C	30, NH
32	-		-			134.9	134.0	C	30, 34, 36
33	7.18	d 8.4	7.36	d 8.7	30, 34	127.5	129.4	CH	30, 37
34	6.74	d 8.4	6.83	d 8.7	33, 38	112.7	114.6	CH	36
35	-		-			157.5	160.3	C	33, 34, 36, 37, 38
36	6.74	d 8.4	6.83	d 8.7	37, 38	112.7	114.6	CH	34
37	7.18	d 8.4	7.36	d 8.7	30, 36	127.5	129.4	CH	30, 33
38	3.69	s	3.75	s	34, 36	55.0	55.7	CH <sub>3</sub>	
39	3.03	s	3.16	s	5, 6 $\alpha$ , 9, 12 $\alpha$ , 15 $\alpha$	53.5	54.6	CH <sub>3</sub>	
NH	7.78	d 5.0						-	

**Table S3.** Conformational analysis of (24*S*,30*S*)-**1** at the B3LYP/6-31G\*\* level in the gas phase.

# <sup>a</sup>	$\Delta E$ <sup>b</sup>	P% <sup>c</sup>
1	10.20	1.6
2	11.63	0.9
3	34.93	0.0
4	26.12	0.0
5	32.90	0.0
6	26.12	0.0
7	0.00	97.5
8	26.12	0.0
9	27.92	0.0

<sup>a</sup>: conformer number; <sup>b</sup>: relative energy, zero point vibrational energy was included; <sup>c</sup>: conformational distribution.

**Table S4.** Important transition states, related rotatory strengths, and oscillator strengths of (24*S*,30*S*)-**1** at the B3LYP/6-31G\* level in the gas phase.

Transitions	$\Delta E$ <sup>a</sup> (eV)	$\lambda$ <sup>b</sup> (nm)	$f$ <sup>c</sup>	$R_{len}$ <sup>d</sup>
183→186, 180→186	4.82	257.0	0.005	−12.58
182→187, 183→188	5.37	230.9	0.049	38.82
183→188, 182→187	5.39	230.2	0.110	60.84
182→188	5.57	222.5	0.027	9.35
178→186, 176→186, 180→187, 179→186	5.72	216.9	0.022	5.06
180→187, 178→186, 176→186	5.75	215.6	0.039	−24.97
181→188, 183→189, 180→188, 180→187	5.82	212.9	0.004	−14.31
183→189, 180→188	5.88	210.8	0.010	−7.00
178→188, 179→188, 179→186, 176→188	6.04	205.2	0.006	−12.20
182→189, 176→188	6.15	201.6	0.198	83.36
182→189	6.16	201.3	0.172	−136.69
184→190	6.17	200.9	0.005	−5.32

<sup>a</sup> Excited energy; <sup>b</sup> Wavelength; <sup>c</sup> Oscillator strength; <sup>d</sup> Rotatory strength in length form ( $10^{-40}$ cgs).

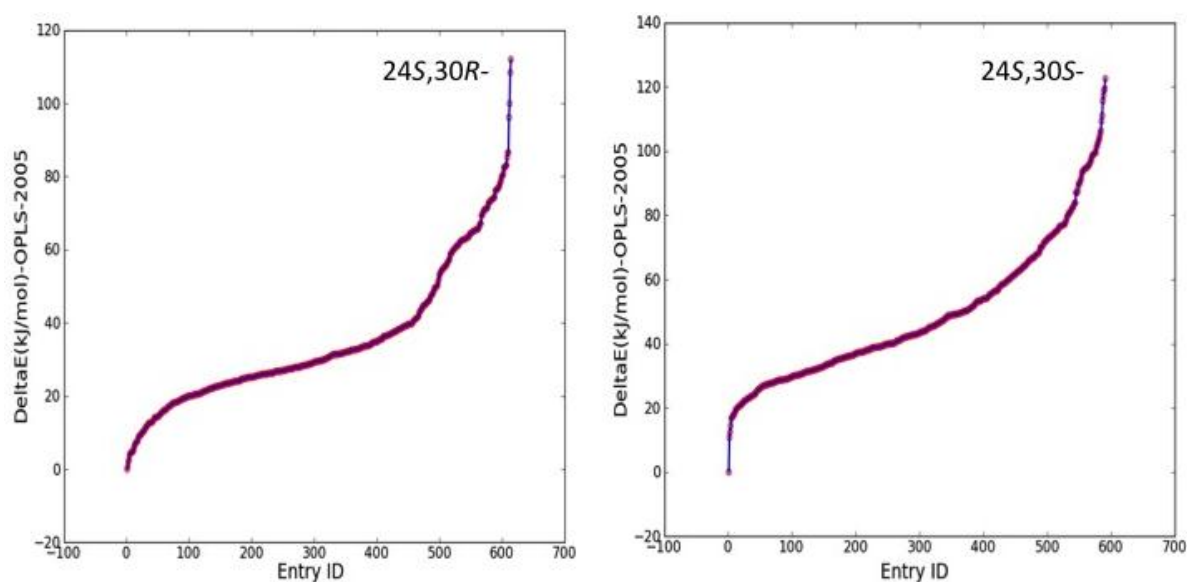
**Table S5.** Experimental and calculated NMR chemical shifts of **1**.

No. <sup>a</sup>	Atom <sup>b</sup>	$\delta_c$ <sup>c</sup>	24 <i>S</i> ,30 <i>S</i>		24 <i>R</i> ,30 <i>S</i>		$\delta_i$ <sup>f</sup>
			$\delta_c$ <sup>d</sup>	$\Delta$ <sup>e</sup>	$\delta_c$ <sup>d</sup>	$\Delta$ <sup>e</sup>	
1	C	35.8	40.1	4.3	40.5	4.7	0.4
2	C	28.2	31.9	3.7	32.5	4.3	0.6
3	C	80.1	75.6	4.5	76.0	4.1	0.4
4	C	37.2	40.7	3.5	41.0	3.8	0.3
5	C	50.7	51.4	0.7	51.6	0.9	0.2
6	C	24.7	24.8	0.1	25.0	0.3	0.1
7	C	29.2	31.8	2.6	31.8	2.6	0.0
8	C	125.9	131.2	5.3	132.6	6.7	1.4
9	C	48.7	55.9	7.2	56.6	7.9	0.6
10	C	36.9	39.7	2.8	39.5	2.6	0.2
11	C	19.5	23.3	3.8	24.4	4.9	1.1

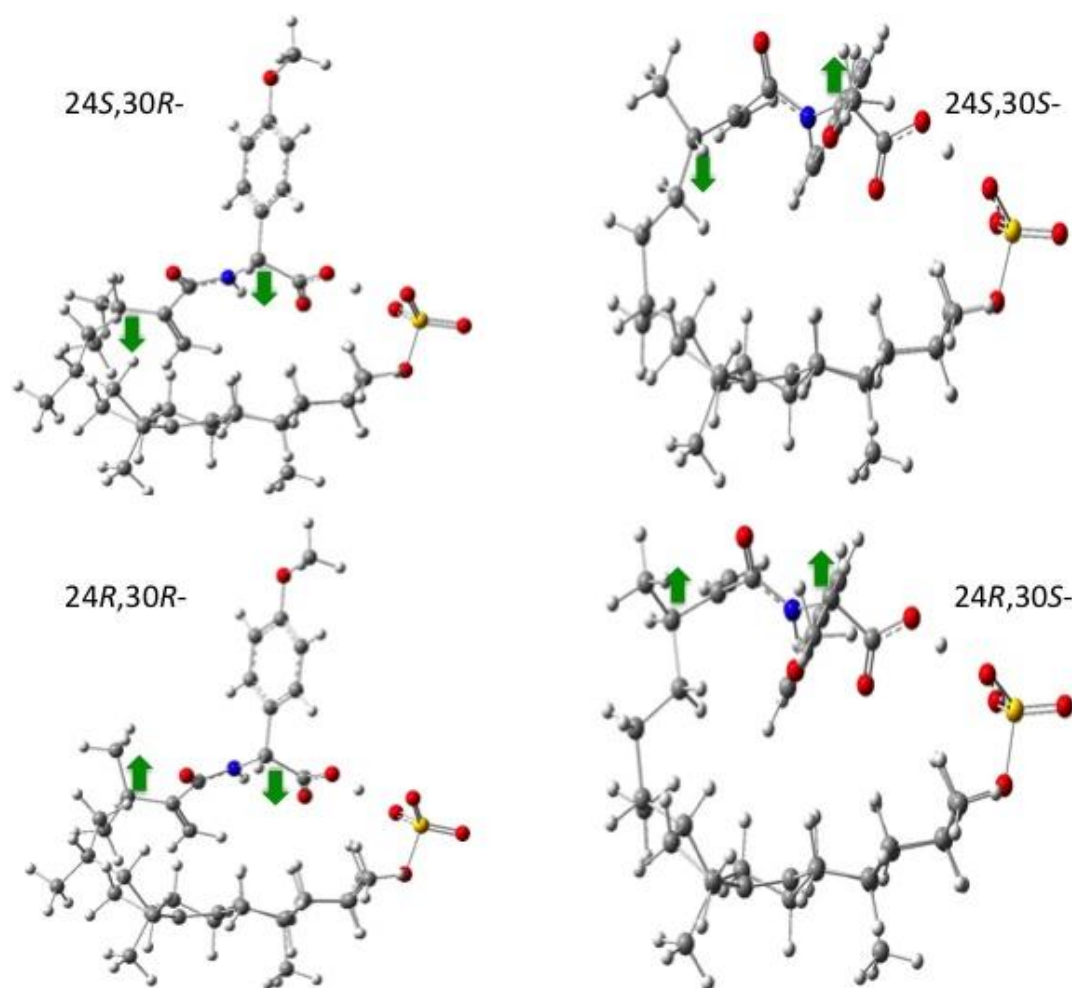
Table S5. Cont.

12	C	36.9	40.0	3.1	41.4	4.5	1.5
13	C	42.2	47.5	5.3	47.7	5.5	0.2
14	C	141.4	136.7	4.7	136.9	4.5	0.2
15	C	25.3	27.4	2.1	27.5	2.2	0.2
16	C	26.6	32.4	<b>5.8</b>	31.6	5.0	0.8
17	C	56.3	54.2	2.1	52.0	4.3	2.2
18	C	18.1	20.5	2.4	20.3	2.2	0.1
19	C	13.7	17.0	3.3	17.5	3.8	0.5
20	C	34.1	39.7	<b>5.6</b>	39.4	5.3	0.2
21	C	19.0	16.9	2.1	19.3	0.3	2.4
22	C	32.5	36.5	4.0	35.0	2.5	1.5
23	C	31.3	33.0	1.7	34.9	3.6	1.9
24	C	35.0	43.1	8.1	48.4	13.4	5.3
25	C	151.4	155.0	3.6	152.6	1.2	2.3
26	C	113.9	106.2	<b>7.7</b>	107.4	<b>6.5</b>	1.2
27	C	166.7	161.2	5.5	159.9	6.8	1.3
<b>28</b>	<b>C</b>	<b>19.7</b>	<b>22.7</b>	<b>3.0</b>	<b>18.0</b>	<b>1.7</b>	<b>4.7</b>
29	C	15.5	15.6	0.1	16.0	0.5	0.4
30	C	58.2	59.6	1.4	61.4	3.2	1.8
31	C	170.4	163.2	<b>7.2</b>	164.8	<b>5.6</b>	1.5
32	C	134.9	128.6	<b>6.3</b>	130.9	<b>4.0</b>	2.2
33	C	127.5	125.8	1.7	126.5	1.0	0.8
34	C	112.7	103.6	<b>9.1</b>	103.8	<b>8.9</b>	0.2
35	C	157.5	150.8	<b>6.7</b>	151.3	<b>6.2</b>	0.5
36	C	112.7	110.8	1.9	111.7	1.0	0.9
37	C	127.5	119.5	<b>8.0</b>	120.3	<b>7.2</b>	0.8
38	C	55.0	52.0	3.0	52.0	3.0	0.1

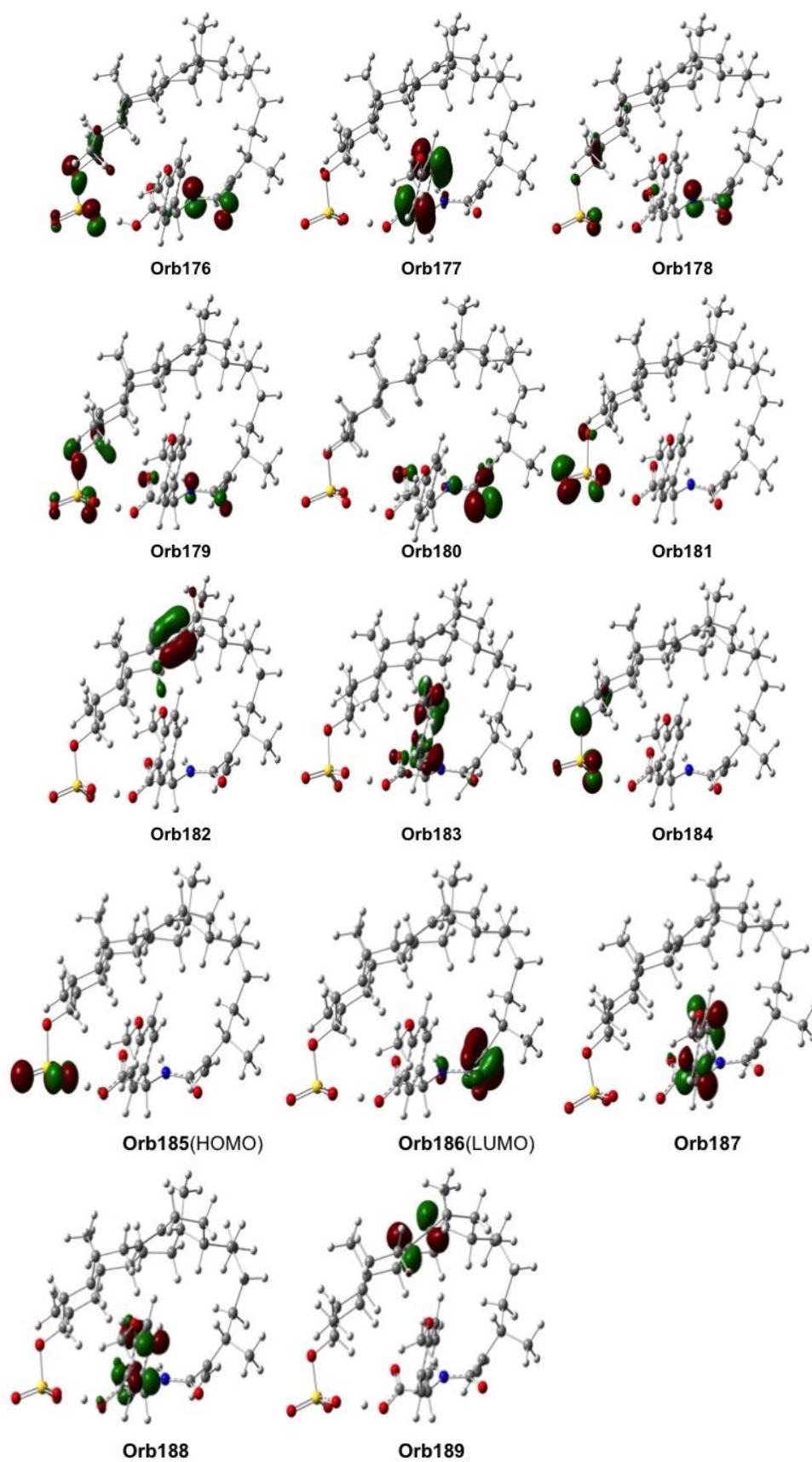
<sup>a</sup> Atom numbering; <sup>b</sup> atom name; <sup>c</sup> Experimentally and <sup>d</sup> Theoretically observed chemical shifts; <sup>e</sup> Difference between experimentally and theoretically observed chemical shifts; <sup>f</sup> Difference between calculated chemical shifts of two configurations. Calculation was performed at the B3LYP/6-31G\*\* level in the gas phase.



**Figure S1.** Random conformational search of (24S,30R) and (24S,30S)-1 with an energy window of 130 kJ/mol.

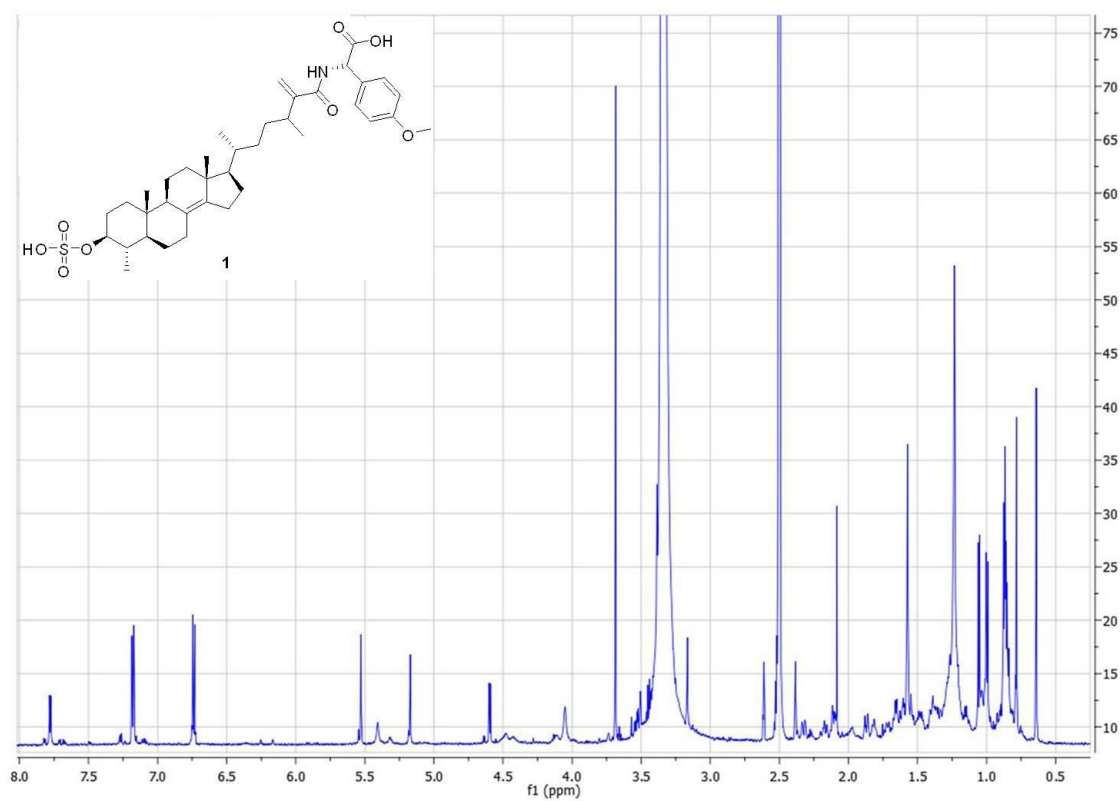


**Figure S2.** Optimized geometries of predominant conformers of 1 at the B3LYP/6-31G\*\* level in the gas phase.

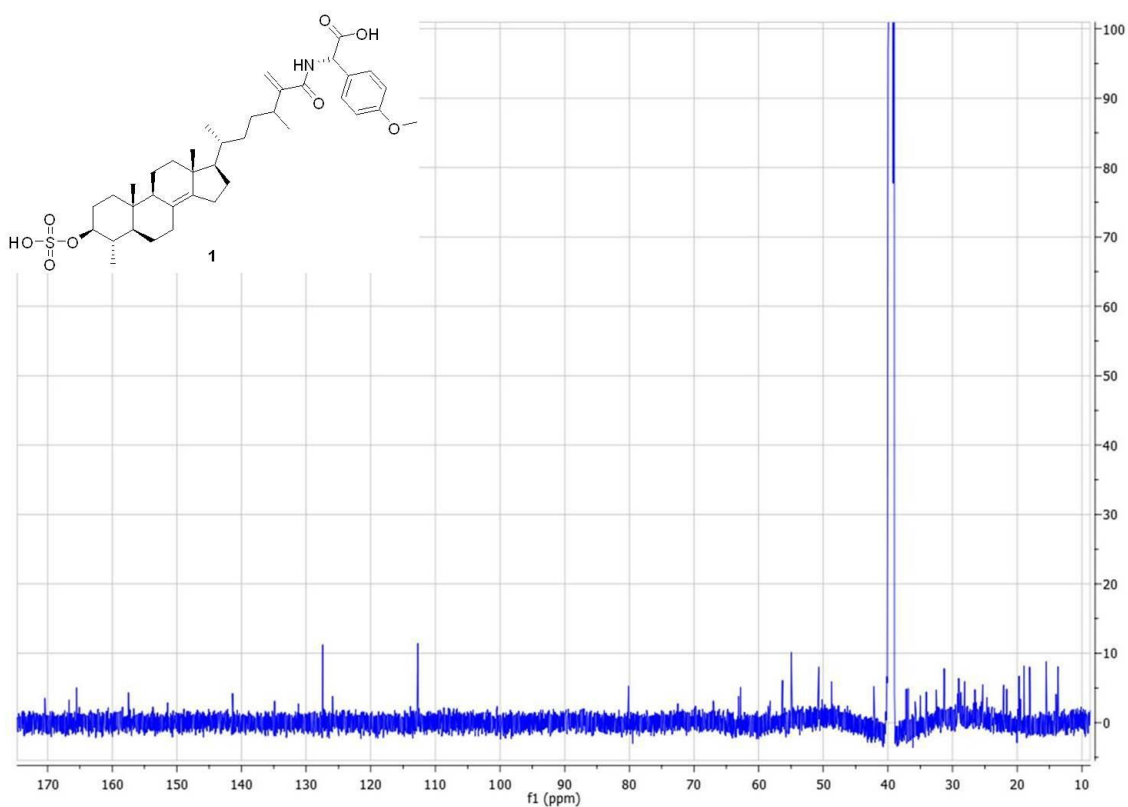


**Figure S3.** Molecular orbitals involved in the key transitions in the calculated ECD spectrum of (24*S*,30*S*)-**1** at the B3LYP/6-31G\*\* level in the gas phase.

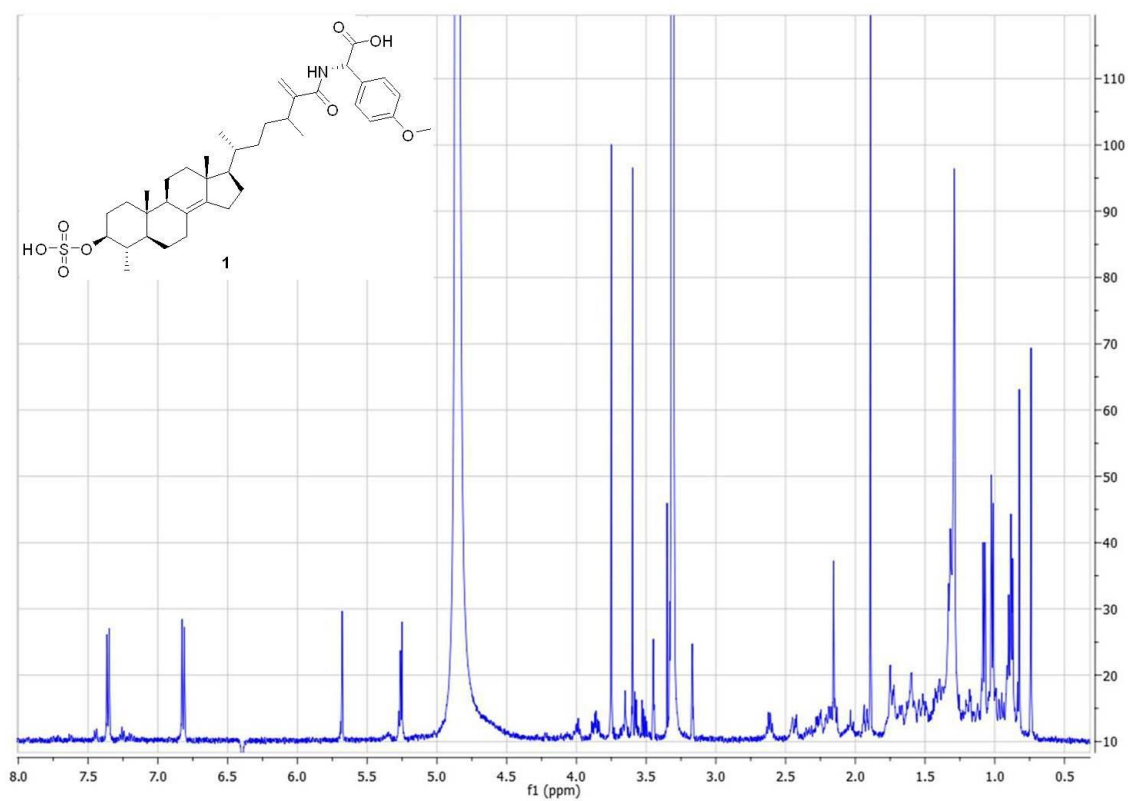




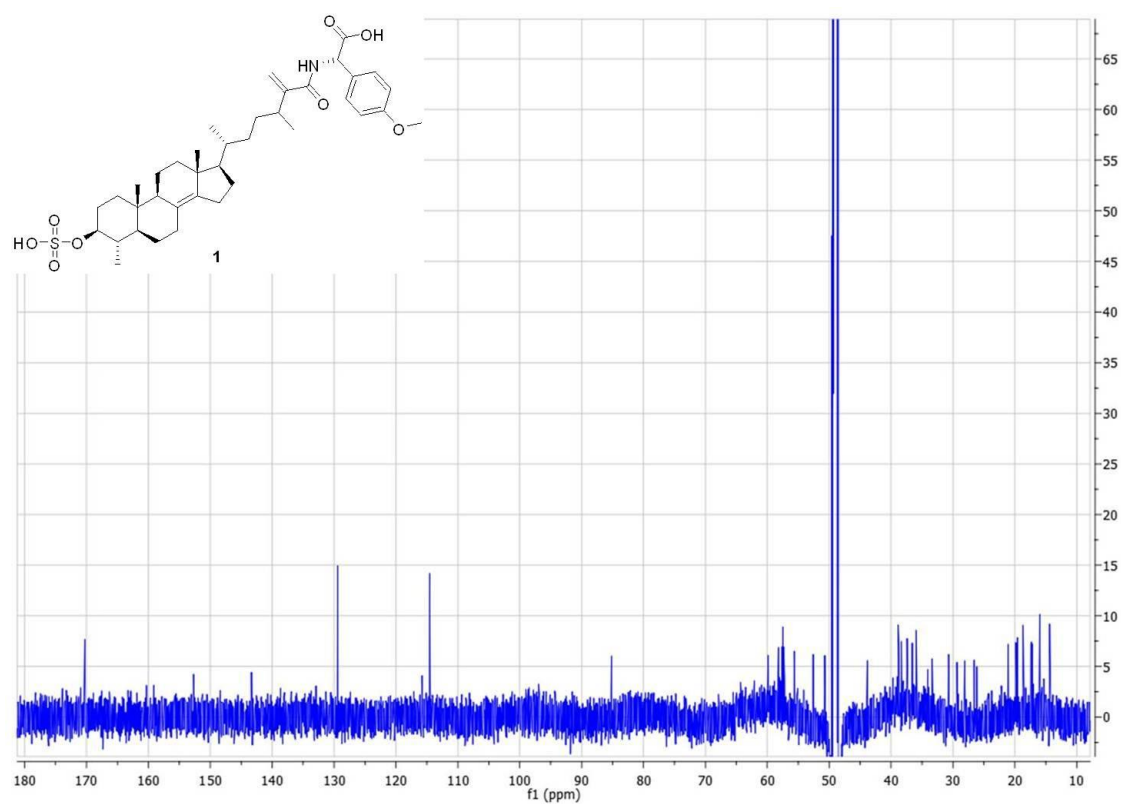
**Figure S4.** <sup>1</sup>H-NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound **1**.



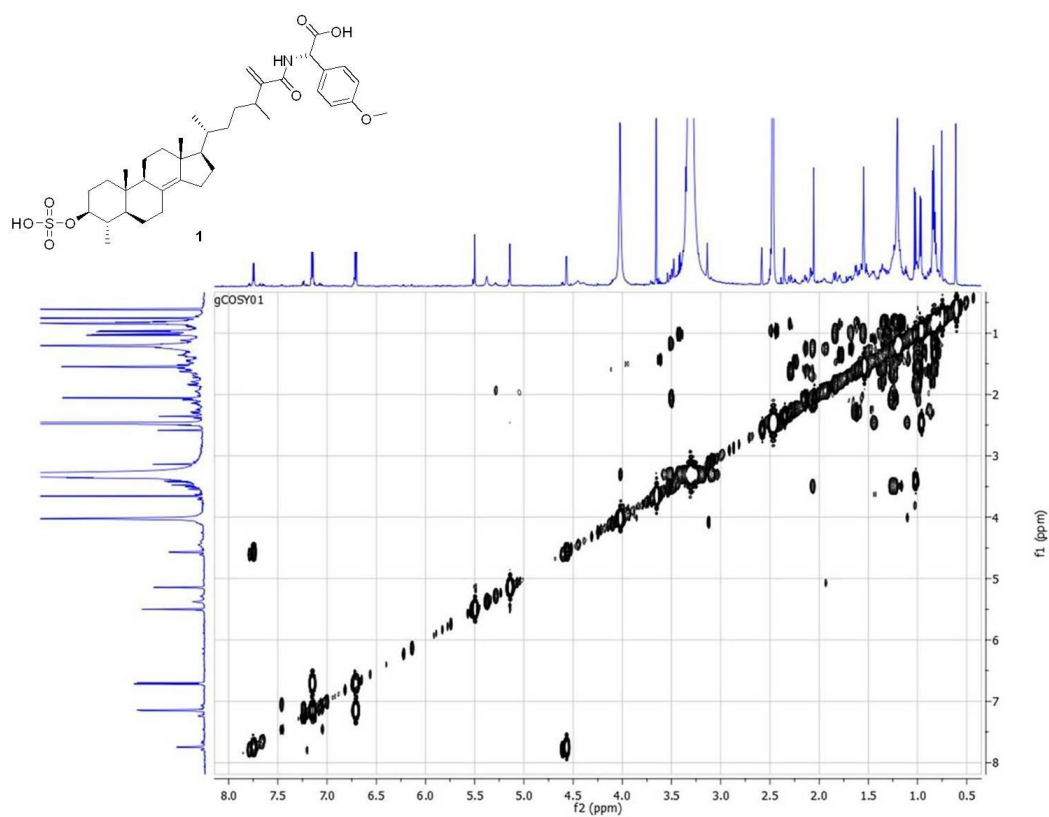
**Figure S5.** <sup>13</sup>C-NMR spectrum (150 MHz, DMSO-*d*<sub>6</sub>) of compound **1**.



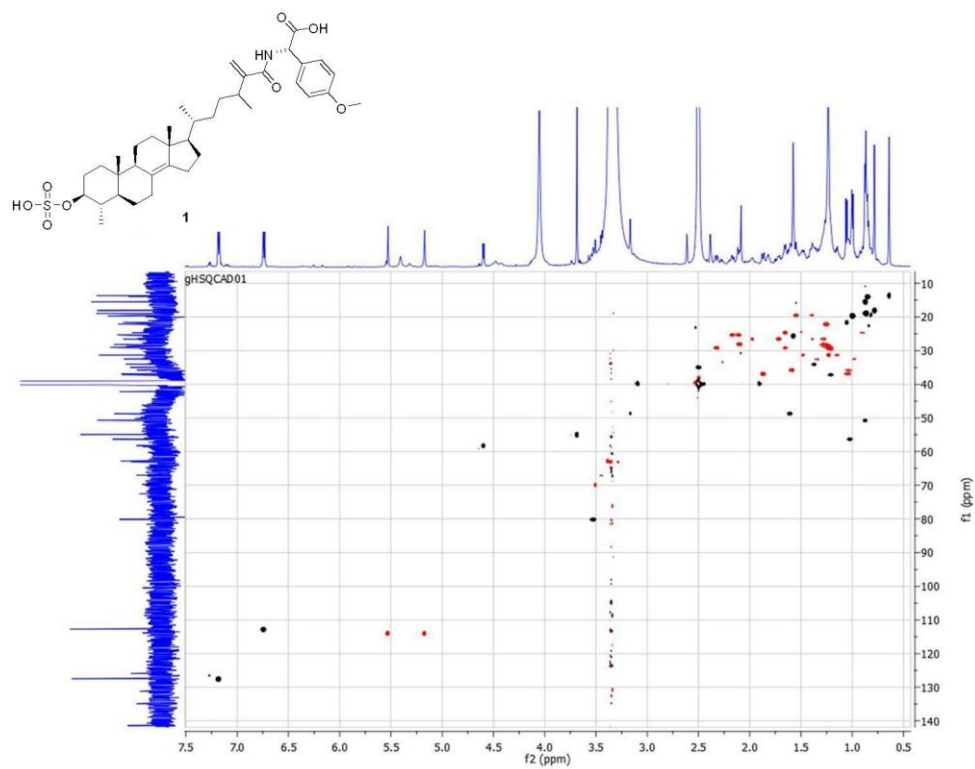
**Figure S6.**  $^1\text{H}$ -NMR spectrum (600 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**.



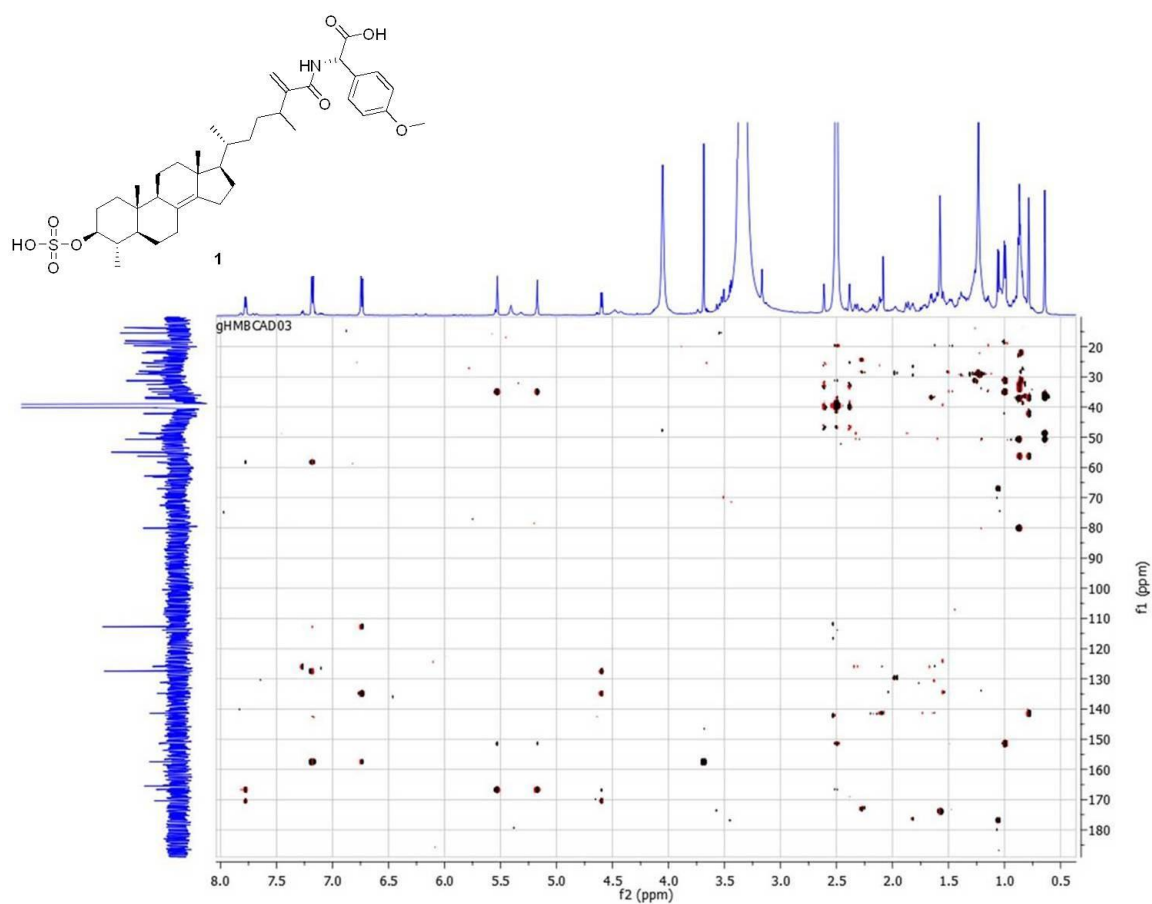
**Figure S7.**  $^{13}\text{C}$  NMR spectrum (150 MHz,  $\text{CD}_3\text{OD}$ ) of compound **1**.



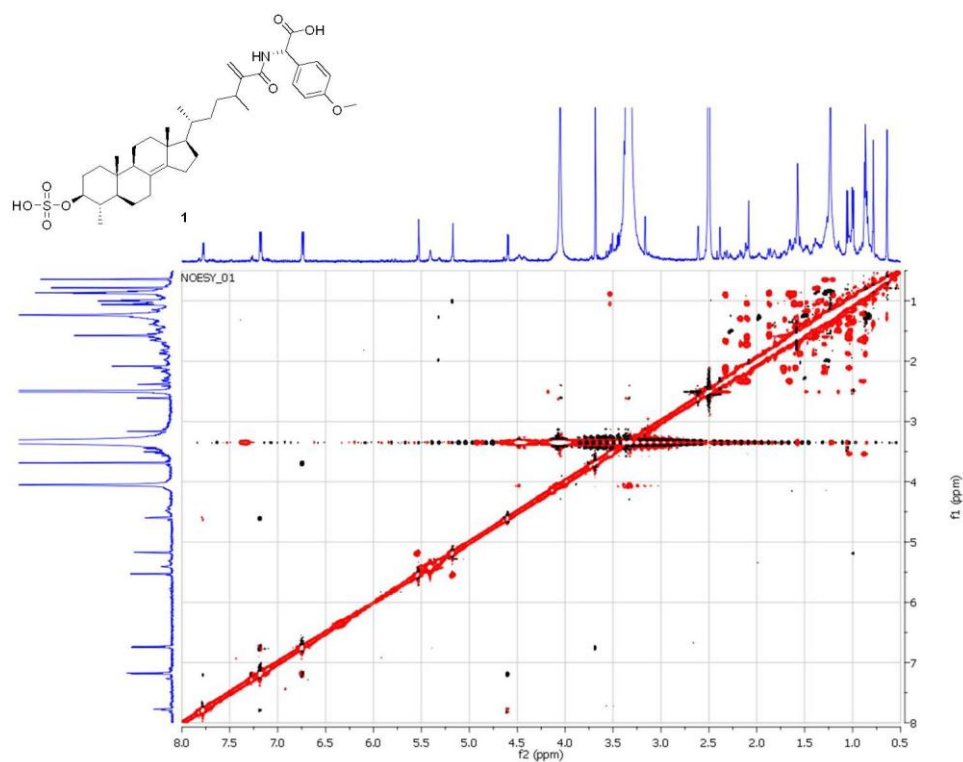
**Figure S8.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (DMSO- $d_6$ ) of compound **1**.



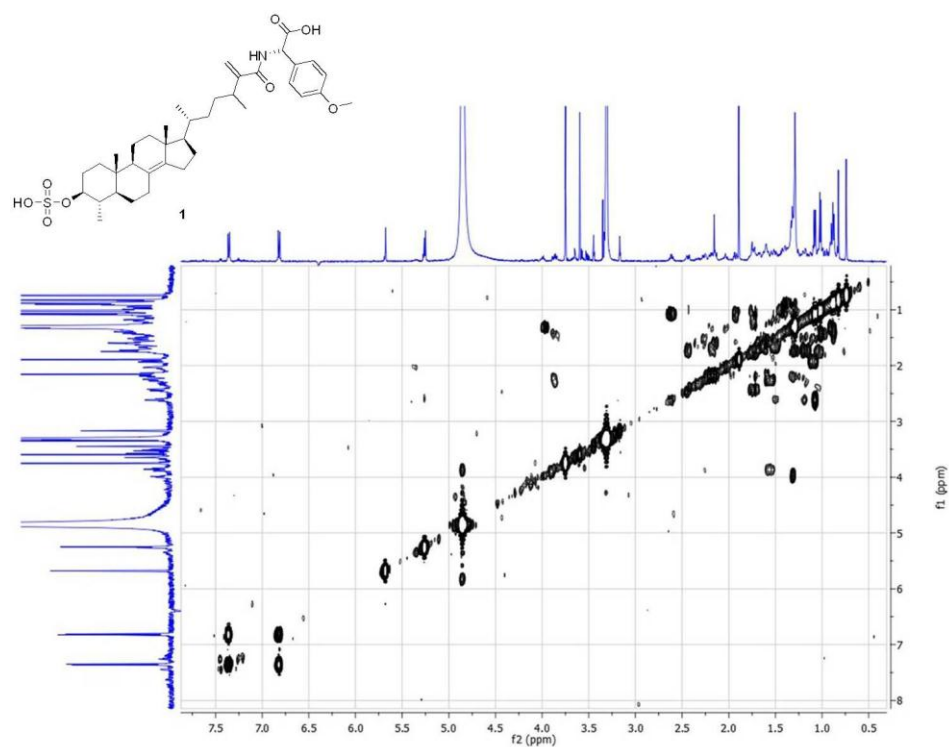
**Figure S9.** HSQC spectrum (DMSO- $d_6$ ) of compound **1**.



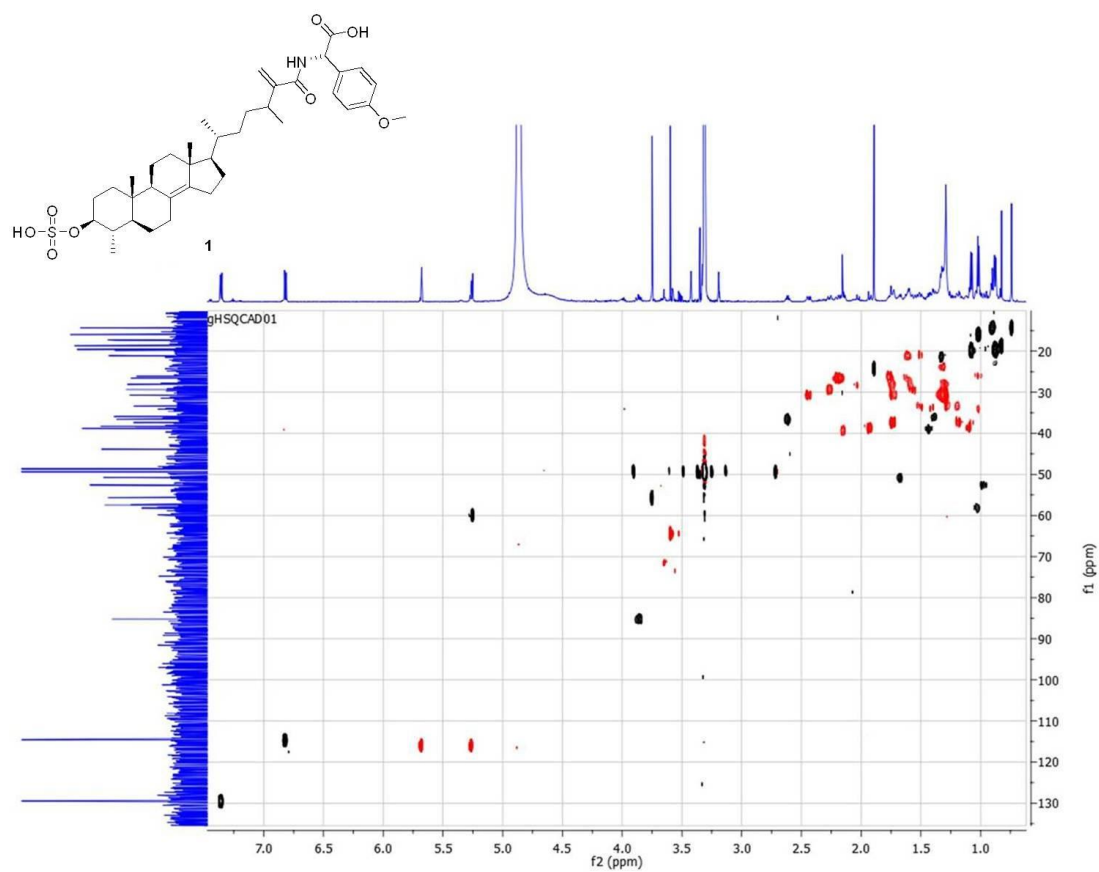
**Figure S10.** HMBC spectrum (DMSO-*d*<sub>6</sub>) of compound **1**.



**Figure S11.** NOESY spectrum (DMSO-*d*<sub>6</sub>) of compound **1**.



**Figure S12.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_3\text{OD}$ ) of compound **1**.

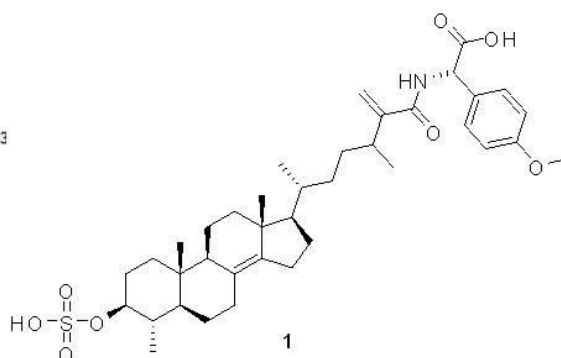


**Figure S13.** HSQC spectrum ( $\text{CD}_3\text{OD}$ ) of compound **1**.

## Qualitative Compound Report

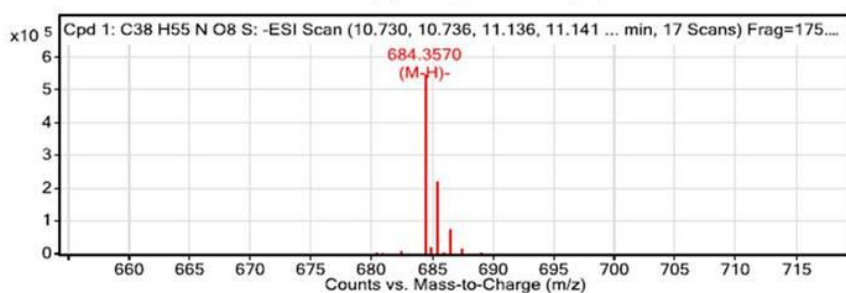
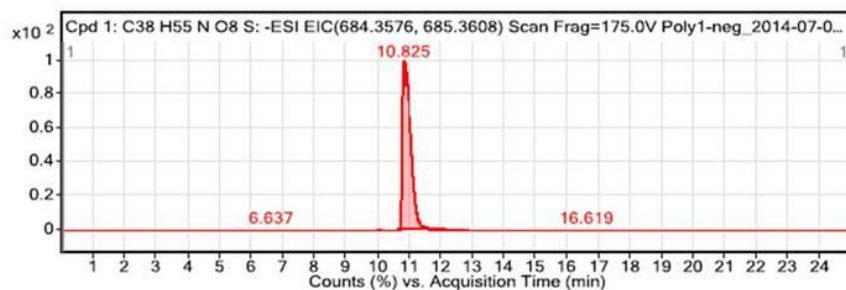
<b>Data File</b>	Poly1-neg_2014-07-01.d	<b>Sample Name</b>	Poly1
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	VsmyNegPoly.m	<b>Acquired Time</b>	01/07/2014 16:06:3
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	Default.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>
<b>Acquisition SW</b>	6200 series TOF/6500 series	
<b>Version</b>	Q-TOF B.05.01 (B5125)	



### Compound Table

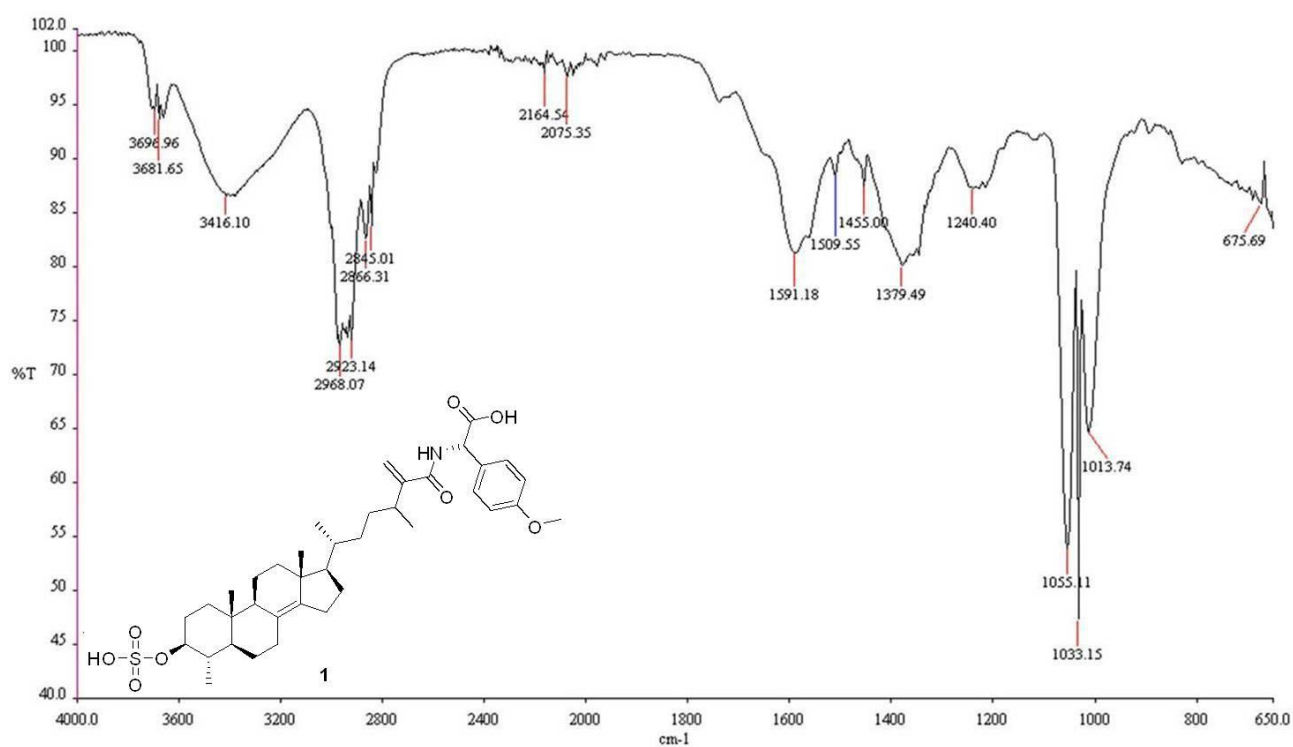
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C38 H55 N O8 S	10.825	685.3646	546887	C38 H55 N O8 S	685.3648	-0.3	C38 H55 N O8 S	C38 H55 N O8 S



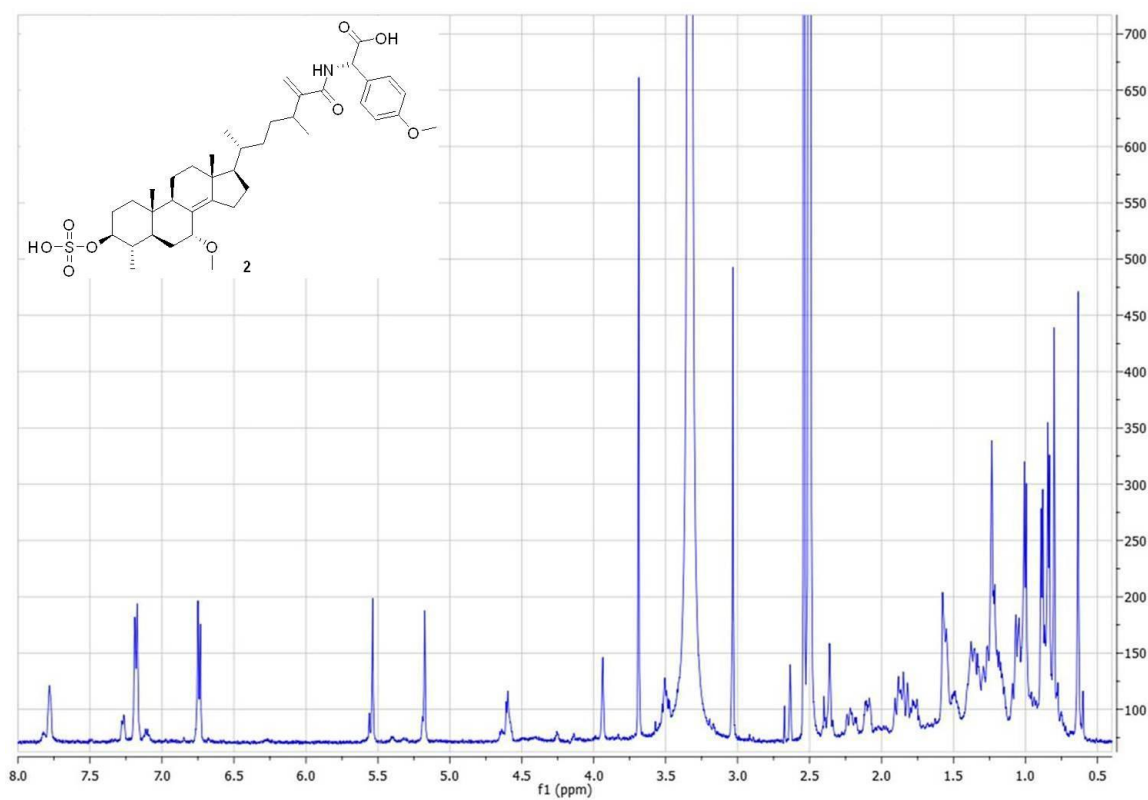
### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Ion
684.357	684.3576	0.75	-1	546886.5	(M-H)-
685.3611	685.3608	-0.34	-1	221727.02	(M-H)-
686.3613	686.3607	-0.81	-1	79107.63	(M-H)-
687.3623	687.3617	-0.84	-1	19181.14	(M-H)-
688.362	688.3632	1.67	-1	4155.32	(M-H)-
689.3617	689.365	4.72	-1	1045.77	(M-H)-

**Figure S14.** ESIMS spectrum of compound 1.

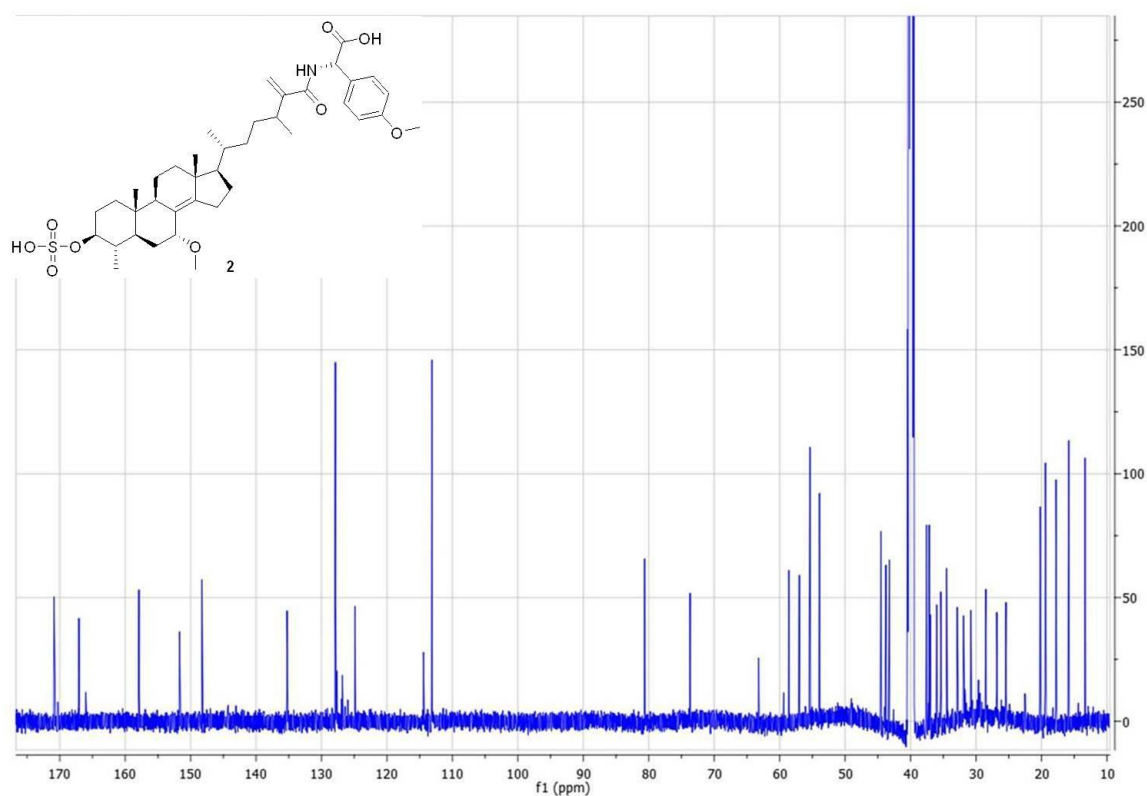


**Figure S15.** IR spectrum of compound 1.

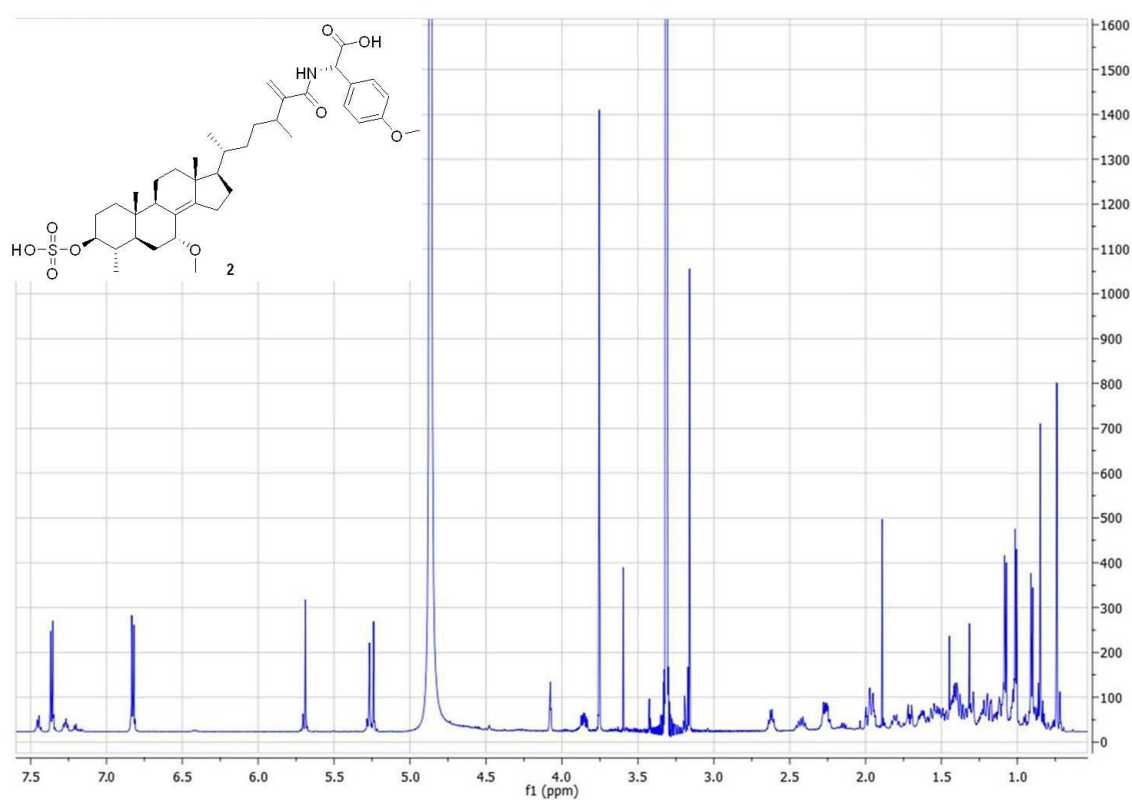


**Figure S16.** <sup>1</sup>H-NMR spectrum (600 MHz, DMSO-*d*<sub>6</sub>) of compound 2.



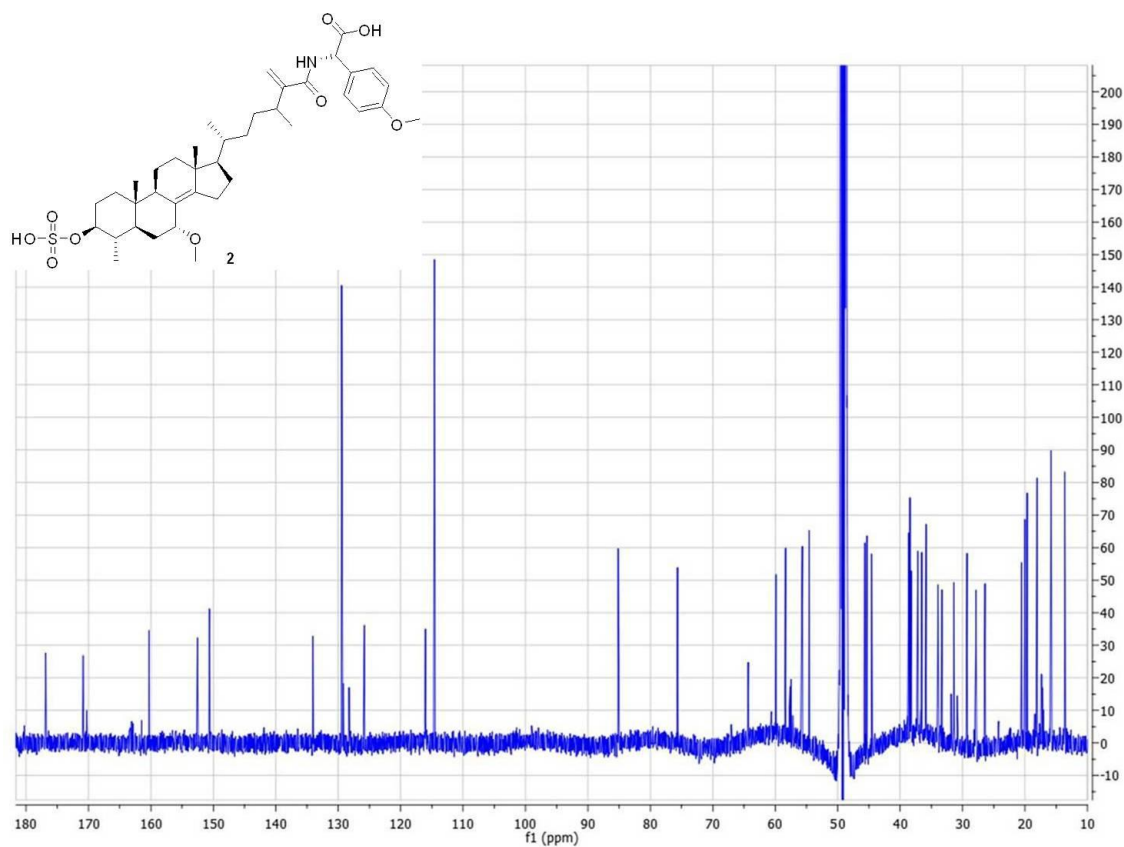


**Figure S17.** <sup>13</sup>C-NMR spectrum (150 MHz, DMSO-*d*<sub>6</sub>) of compound 2.

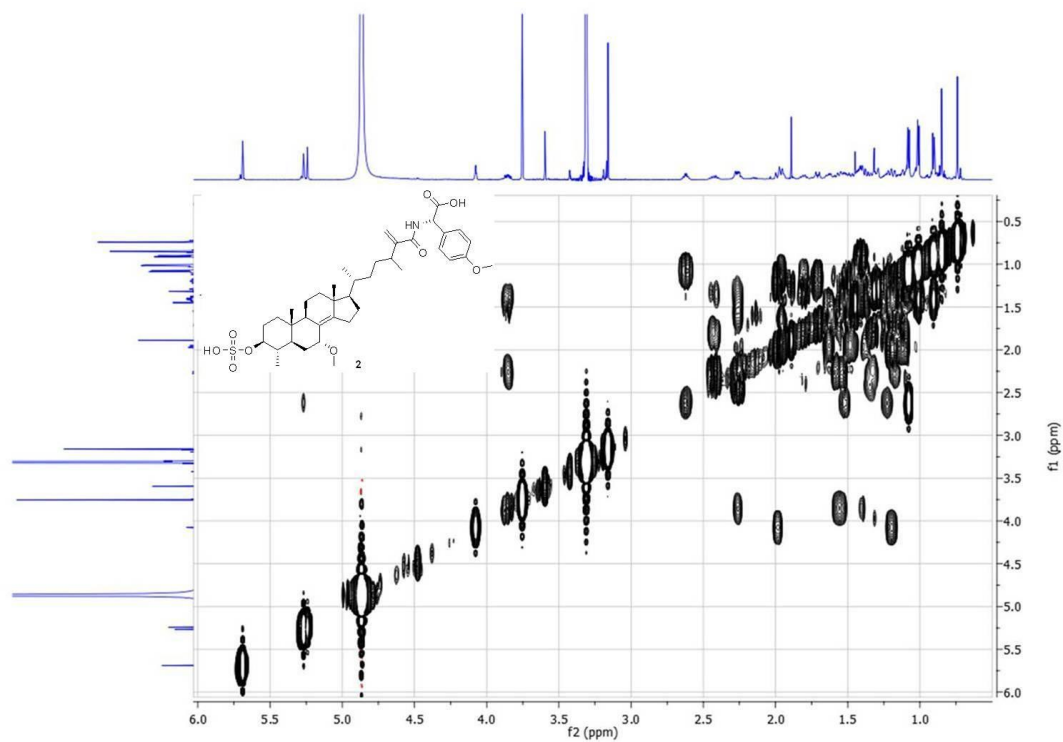


**Figure S18.** <sup>1</sup>H-NMR spectrum (600 MHz, CD<sub>3</sub>OD) of compound 2.

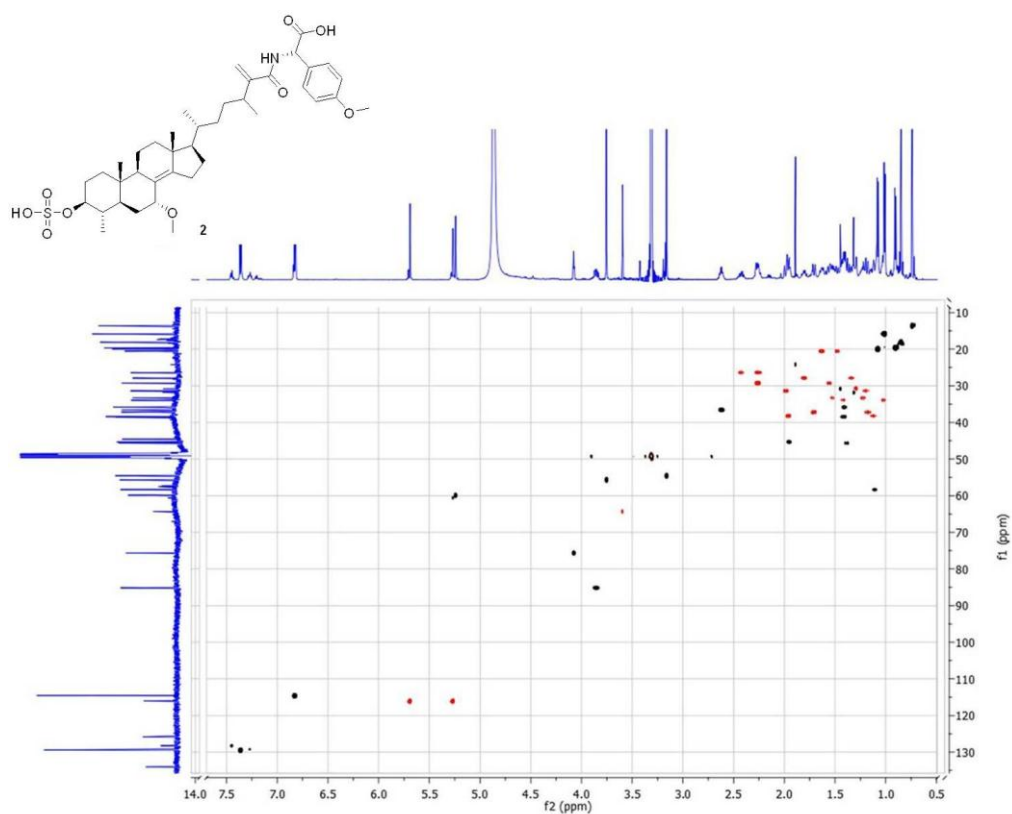




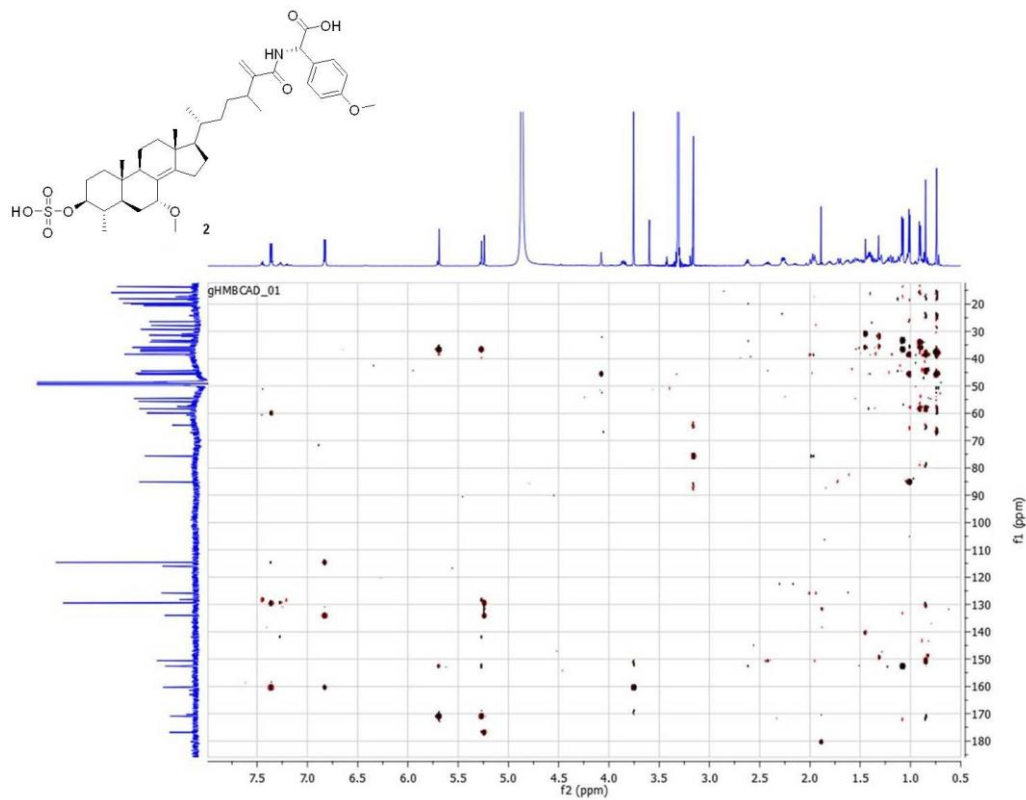
**Figure S19.**  $^{13}\text{C}$ -NMR spectrum (150 MHz,  $\text{CD}_3\text{OD}$ ) of compound 2.



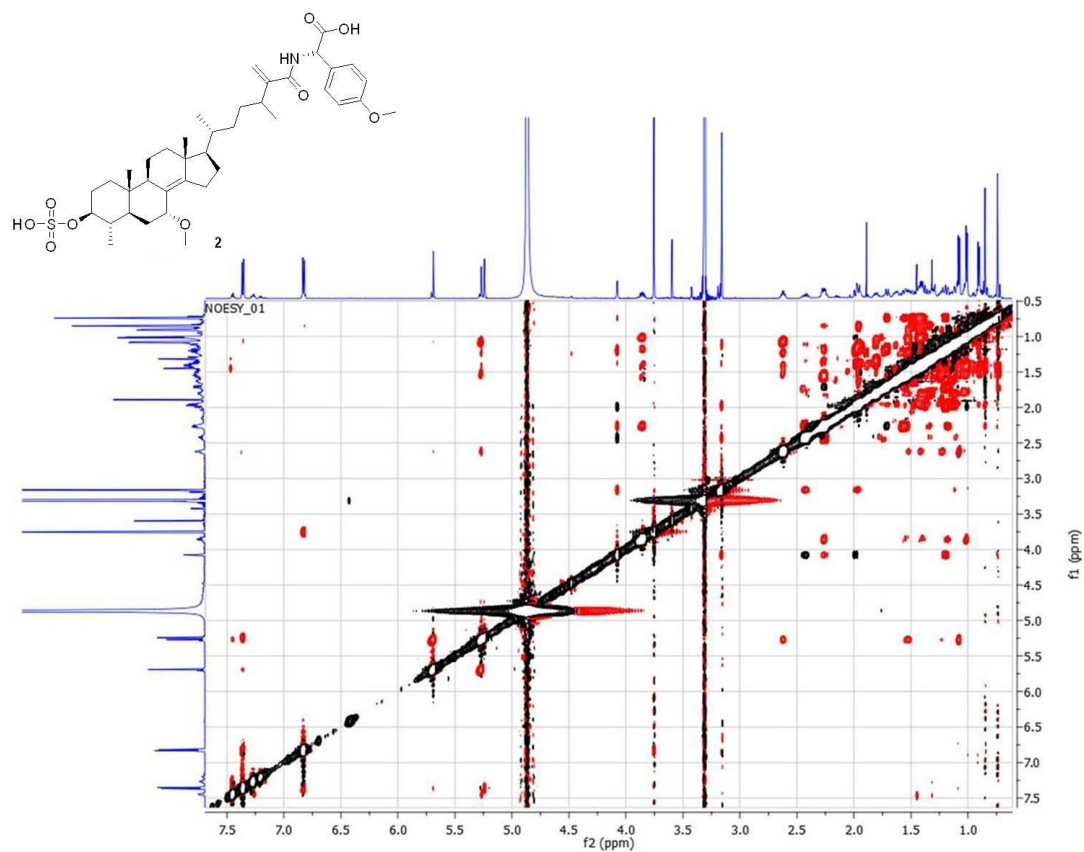
**Figure S20.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_3\text{OD}$ ) of compound 2.



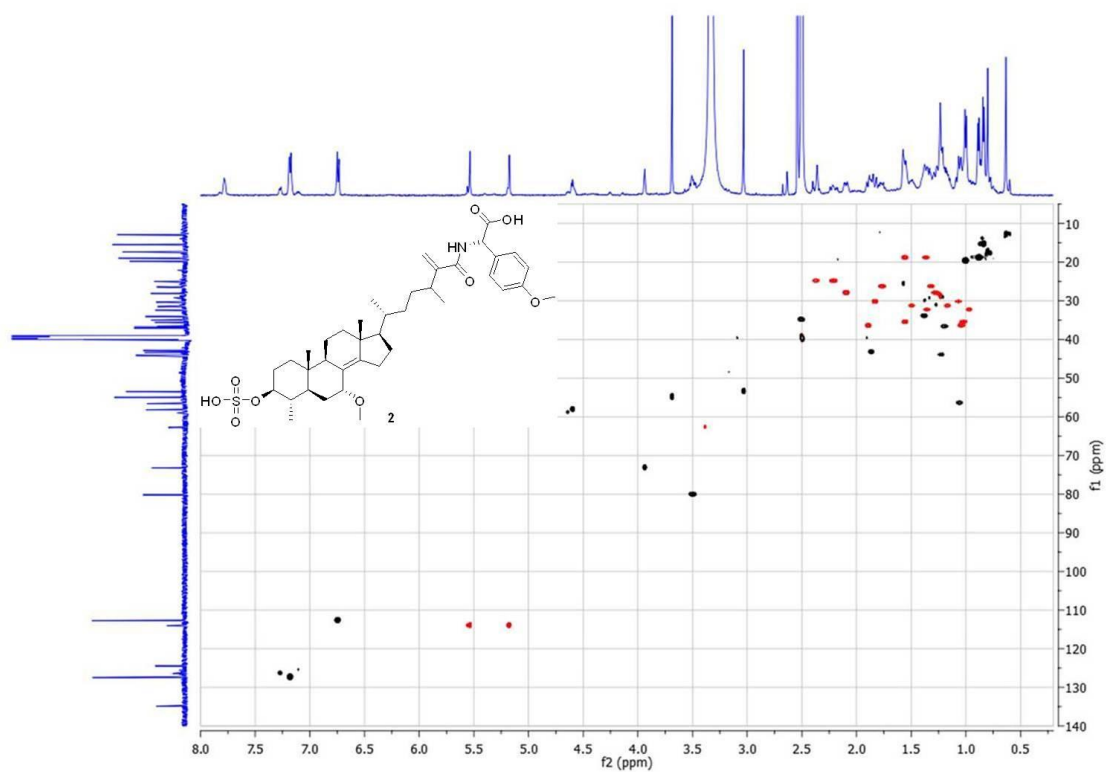
**Figure S21.** HSQC spectrum (CD<sub>3</sub>OD) of compound 2.



**Figure S22.** HMBC spectrum (CD<sub>3</sub>OD) of compound 2.



**Figure S23.** NOESY spectrum (CD<sub>3</sub>OD) of compound 2.



**Figure S24.** HSQC spectrum (DMSO-*d*<sub>6</sub>) of compound 2.

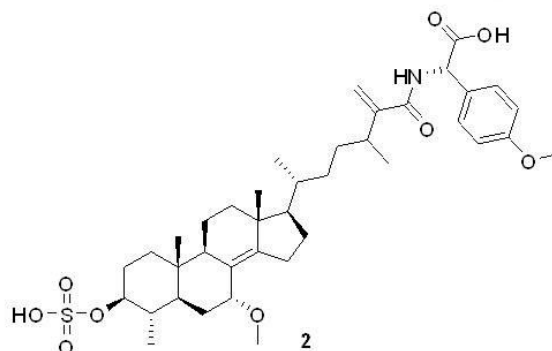
## Qualitative Compound Report

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 Instrument Name Instrument 1  
 Acq Method VsmyNegPoly.m  
 IRM Calibration Status Success  
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 User Name  
 Acquired Time 01/07/2014 17:22:37  
 DA Method Default.m

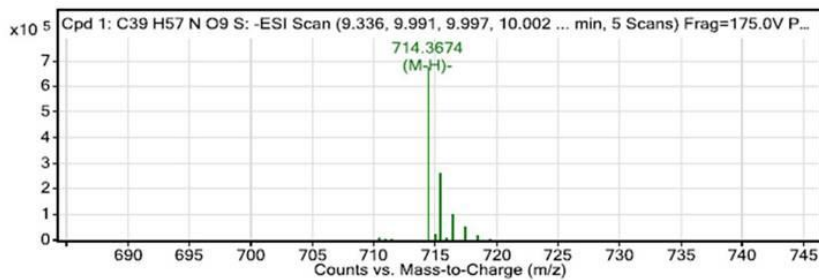
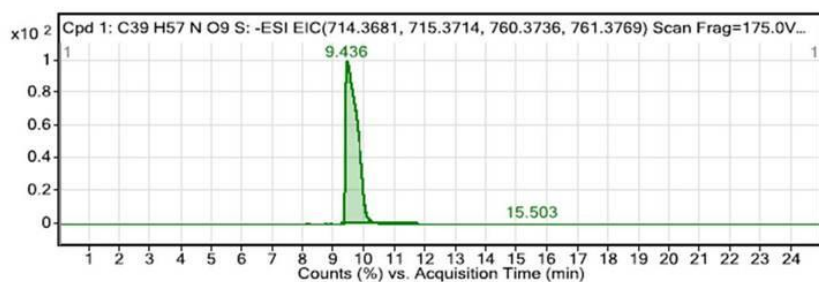
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 Version Q-TOF B.05.01 (B5125)

Info.



## Compound Table

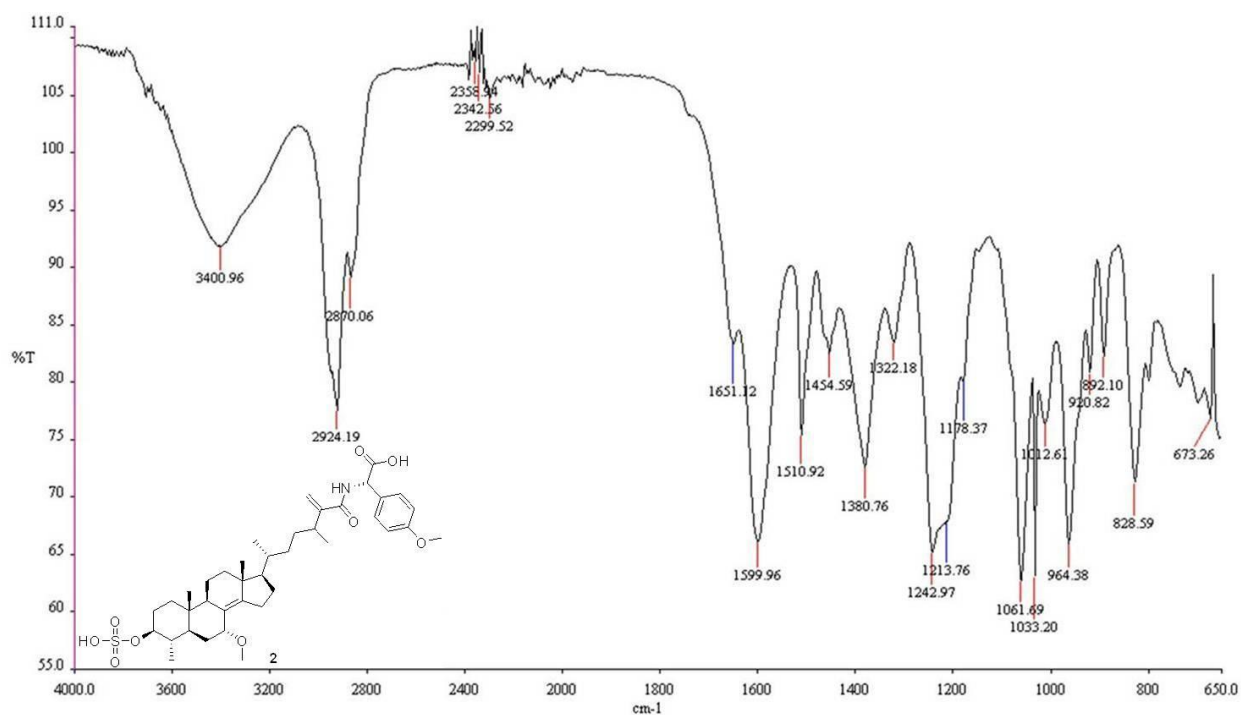
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C <sub>39</sub> H <sub>57</sub> N <sub>1</sub> O <sub>9</sub> S	9.436	715.3749	675238	C <sub>39</sub> H <sub>57</sub> N <sub>1</sub> O <sub>9</sub> S	715.3754	-0.68	C <sub>39</sub> H <sub>57</sub> N <sub>1</sub> O <sub>9</sub> S	C <sub>39</sub> H <sub>57</sub> N <sub>1</sub> O <sub>9</sub> S



## MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Ion
714.3674	714.3681	1.07	-1	675238.25	(M-H) <sup>-</sup>
715.3715	715.3714	-0.08	-1	261685.7	(M-H) <sup>-</sup>
716.3714	716.3714	0.06	-1	103016.8	(M-H) <sup>-</sup>

Figure S25. ESIMS spectrum of compound 2.



**Figure S26.** IR spectrum of compound 2.

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